

Product-form Poisson-like distributions and complex balanced reaction systems

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Abstract

Stochastic reaction networks are dynamical models of biochemical reaction systems and form a particular class of continuous-time Markov chains on \mathbb{N}^n . Here we provide a fundamental characterisation that connects structural properties of a network to its dynamical features. Specifically, we define the notion of ‘stochastically complex balanced systems’ in terms of the network’s stationary distribution and provide a characterisation of stochastically complex balanced systems, parallel to that established in the 70-80ies for deterministic reaction networks. Additionally, we establish that a network is stochastically complex balanced if and only if an associated deterministic network is complex balanced (in the deterministic sense), thereby proving a strong link between the theory of stochastic and deterministic networks. Further, we prove a stochastic version of the ‘deficiency zero theorem’ and show that any (not only complex balanced) deficiency zero reaction network has a product-form Poisson-like stationary distribution on all irreducible components. Finally, we provide sufficient conditions for when a product-form Poisson-like distribution on a single (or all) component(s) implies the network is complex balanced, and explore the possibility to characterise complex balanced systems in terms of product-form Poisson-like stationary distributions.

1 Introduction

Improved experimental techniques have made it possible to measure molecular fluctuations at a small scale, creating a need for a stochastic description of molecular data [24, 12]. Typically, biochemical reaction networks are modelled as deterministic systems of ordinary differential equations (ODEs), but these models assume the individual species are in high concentrations and do not allow for stochastic fluctuation. An alternative is stochastic models based on continuous-time Markov chains [18, 19, 14, 4, 5, 12]. As an example of a stochastic reaction system, consider



where κ_1, κ_2 are positive reaction constants. The network consists of three chemical species A , B and C and two reactions. Each occurrence of a reaction modifies the species counts, for example, when the reaction $A + B \rightarrow 2C$ takes places, the amount of A and B molecules are each decreased by one, while two molecules of C are created. The species counts are modelled as a continuous-time Markov chain, where the transitions are single occurrences of reactions with transition rates

$$\lambda_1(x) = \kappa_1 x_A x_B, \quad \lambda_2(x) = \kappa_2 x_C (x_C - 1),$$

and $x = (x_A, x_B, x_C)$ are the species counts [4]. When modelled deterministically, the concentrations (rather than the counts) of the species change according to an ODE system.

In a classical paper [18], Kurtz explored the relationship between deterministic and stochastic reaction systems, using a scaling argument – large volume limit – to link the dynamical behaviour of the two types of systems to each other. Other, mainly recent work, also points to close connections between the two types of systems [23, 2, 3, 1, 6, 16]. In this paper we explore this relationship further.

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A fundamental link between structural network properties and dynamical features of deterministic reaction networks has been known since the 1970s and 1980s with the work of Horn, Jackson and Feinberg [13, 10]. Specifically, their theory concerns the existence and uniqueness of equilibria in *complex balanced* systems, with the ‘deficiency zero theorem’ playing a central role in this context. Complex balanced systems were called cyclic balanced systems by Boltzmann. They have attractive analytical and physical properties; for example a (pseudo-)entropy might be defined which increases along all trajectories (Boltzmann’s H-theorem) [7, 13].

A parallel theory for the stochastic regime is not available, and the very concept of “complex balanced” does not currently have a stochastic counterpart. In this paper we develop a theory to fill this gap. We define *stochastically complex balanced* systems through properties of the stationary distribution, and we prove results for stochastic reaction networks that are in direct correspondence with the results for deterministic models. In particular, we prove a parallel statement of the deficiency zero theorem and show that all deficiency zero reaction networks have product-form Poisson-like stationary distributions, irrespectively whether they are complexed balanced or not. In fact, in the non-complexed balanced case, the network is complex balanced on the boundary of the state space.

A second target of our study concerns product-form stationary distributions. Such distributions are computationally and analytically tractable and appear in many areas of applied probability, such as, queueing theory [15, 17], Petri Net theory [21], and stochastic reaction network theory [23, 20, 2]. Specifically, a complex balanced mass-action network has a product-form Poisson-like stationary distribution on every irreducible component [20, 2]. As an example, the stationary distribution of the complex balanced reaction system (1.1) is

$$\pi_\Gamma(x) = M_\Gamma \frac{\kappa_1^{x_A} \kappa_2^{x_B} \kappa_1^{x_C}}{x_A! x_B! x_C!} \quad \text{for } x \in \Gamma,$$

where $\Gamma = \{x \in \mathbb{N}^3 : x_A + x_B + 2x_C = \theta\}$ is an irreducible component of the state space \mathbb{N}^3 and M_Γ is a normalising constant.

We expand the above result on mass-action systems and give general conditions under which the converse statement is true. In particular, we are interested in providing a structural characterisation of the networks with product-form Poisson-like stationary distributions. However, this class of networks is strictly larger than that of complex balanced networks, and a full characterisation seems hard to achieve. We illustrate this with examples.

2 Background

We first introduce the necessary notation and background material; see [4, 10, 9] for general references. We assume standard knowledge about continuous-time Markov chains.

2.1 Notation

We let \mathbb{R} , \mathbb{R}_0 and \mathbb{R}_+ be the real, the non-negative real and the positive real numbers, respectively. Also let \mathbb{N} be the natural numbers including 0.

For any real number $a \in \mathbb{R}$, $|a|$ denotes the absolute value of a . Moreover, for any vector $v \in \mathbb{R}^p$, we let v_i be the i th component of v , $\|v\|$ the Euclidean norm, and $\|v\|_\infty$ the infinity norm, that is, $\|v\|_\infty = \max_i |v_i|$. For two vectors $v, w \in \mathbb{R}^p$, we write $v < w$ (resp. $v > w$) and $v \leq w$ (resp. $v \geq w$), if the inequality holds component-wise. Further, we define $\mathbb{1}_{\{v \leq w\}}$ to be one if $v \leq w$, and zero otherwise, and similarly for the other inequalities. If $v > 0$ then v is said to be positive. Finally, $\text{supp } v$ denotes the index set of the non-zero components. For example, if $v = (0, 1, 1)$ then $\text{supp } v = \{2, 3\}$.

If $x \in \mathbb{R}_0^q$ and $v \in \mathbb{N}^q$, we define

$$x^v = \prod_{i=1}^q x_i^{v_i}, \quad \text{and} \quad v! = \prod_{i=1}^q v_i!,$$

with the conventions that $0! = 1$ and $0^0 = 1$.

2.2 Reaction networks

A reaction network is a triple $\mathcal{G} = (\mathcal{X}, \mathcal{C}, \mathcal{R})$, where $\mathcal{X} = \{S_1, S_2, \dots, S_n\}$ is a set of n species, \mathcal{C} is a set of m complexes, and $\mathcal{R} \subseteq \mathcal{C} \times \mathcal{C}$ is a set of k reactions, such that $(y, y) \notin \mathcal{R}$ for all $y \in \mathcal{C}$. The complexes are linear combinations of species on \mathbb{N} , identified as vectors in \mathbb{R}^n . A reaction $(y, y') \in \mathcal{R}$ is denoted by $y \rightarrow y'$. We require that every species is part of at least one complex, and that every complex is part of at least one reaction. In this way, there are no “superfluous” species or complexes and \mathcal{G} is completely determined by the set of reactions \mathcal{R} , which we allow to be empty. In (1.1), there are $n = 3$ species (A, B, C) , $m = 2$ complexes $(A + B, 2C)$, and $k = 2$ reactions.

Given a reaction network \mathcal{G} , the *reaction graph* of \mathcal{G} is the directed graph with node set \mathcal{C} and edge set \mathcal{R} . We let ℓ be the number of linkage classes (connected components) of the reaction graph. A reaction $y \rightarrow y' \in \mathcal{R}$ is *terminal* if any directed path that starts with $y \rightarrow y'$ is contained in a closed directed path. We let \mathcal{R}^* be the set of terminal reactions.

A reaction network \mathcal{G} is *weakly reversible*, if every reaction is terminal. The network in (1.1) is weakly reversible, since both reactions are terminal.

The *stoichiometric subspace* of \mathcal{G} is the linear subspace of \mathbb{R}^n given by

$$S = \text{span}(y' - y | y \rightarrow y' \in \mathcal{R}).$$

For $v \in \mathbb{R}^n$, the sets $(v + S) \cap \mathbb{R}_0^n$ are called the *stoichiometric compatibility classes* of \mathcal{G} (Fig. 1A). For the network in (1.1), $S = \text{span}((-1, 1, 0), (0, 1, -1)) \subset \mathbb{R}^3$, which is 2-dimensional.

2.3 Dynamical systems

We will consider a reaction network \mathcal{G} either as a deterministic dynamical system on the continuous space \mathbb{R}_0^n , or as a stochastic dynamical system on the discrete space \mathbb{N}^n .

In the deterministic case, the evolution of the species concentrations $z = z(t) \in \mathbb{R}_0^n$ at time t is modelled as the solution to the ODE

$$\frac{dz}{dt} = \sum_{y \rightarrow y' \in \mathcal{R}} (y' - y) \lambda_{y \rightarrow y'}(z), \quad (2.1)$$

for some functions $\lambda_{y \rightarrow y'}: \mathbb{R}_0^n \rightarrow \mathbb{R}_0$ and an initial condition $z(0) \in \mathbb{R}_0^n$. We require that the functions $\lambda_{y \rightarrow y'}$ are continuously differentiable, and that $\lambda_{y \rightarrow y'}(z) > 0$ if and only if $\text{supp } y \subseteq \text{supp } z$. Such functions are called *rate functions*, they constitute a *deterministic kinetics* K for \mathcal{G} , and the pair (\mathcal{G}, K) is called a *deterministic reaction system*. If $\lambda_{y \rightarrow y'}(z) = \kappa_{y \rightarrow y'} z^y$ for all reactions, then the constants $\kappa_{y \rightarrow y'}$ are referred to as *rate constants* and the modelling regime is referred to as *deterministic mass-action kinetics*. In this case, the pair (\mathcal{G}, κ) is called a *deterministic mass-action system*, where $\kappa \in \mathbb{R}_+^k$ is the vector of rate constants.

In the stochastic setting, the evolution of the species counts $X(t) \in \mathbb{N}^n$ at time t is modelled as a continuous-time Markov chain with state space \mathbb{N}^n . At any state $x \in \mathbb{N}^n$, the states that can be reached in one step are $x + y' - y$ for $y \rightarrow y' \in \mathcal{R}$, with transition rates $\lambda_{y \rightarrow y'}(x)$. The functions $\lambda_{y \rightarrow y'}: \mathbb{N}^n \rightarrow \mathbb{R}_0$ are called *rate functions*, and we require that $\lambda_{y \rightarrow y'}(x) > 0$ if and only if $x \geq y$. A choice of these functions constitute a *stochastic kinetics* K for \mathcal{G} and the pair (\mathcal{G}, K) is called a *stochastic reaction system*. If the reaction $y \rightarrow y'$ occurs at time t , then the new state is

$$X(t) = X(t-) + y' - y,$$

where $X(t-)$ denotes the previous state. If for any reaction $y \rightarrow y' \in \mathcal{R}$

$$\lambda_{y \rightarrow y'}(x) = \kappa_{y \rightarrow y'} \frac{x!}{(x - y)!} \mathbb{1}_{\{x \geq y\}},$$

then the constants $\kappa_{y \rightarrow y'}$ are known as *rate constants*, as in the deterministic case, and the modelling regime is referred to as *stochastic mass-action kinetics*. The pair (\mathcal{G}, κ) is, in this case, called a *stochastic mass-action system*.

The evolution of the stochastic as well as the deterministic reaction system is confined to the stoichiometric compatibility classes,

$$z(t) \in (z(0) + S) \cap \mathbb{R}_0^n \quad \text{and} \quad X(t) \in (X(0) + S) \cap \mathbb{N}_0^n.$$

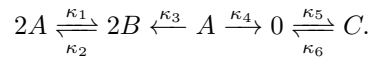
In fact, $X(t) \in (X(0) + S) \cap \mathbb{N}^n$, as $X(t)$ takes values in \mathbb{N}^n .

Definition 1. Let $\mathcal{G} = (\mathcal{X}, \mathcal{C}, \mathcal{R})$ be a reaction network.

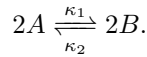
- a) A reaction network $\mathcal{G}' = (\mathcal{X}', \mathcal{C}', \mathcal{R}')$ is a subnetwork of \mathcal{G} if $\mathcal{R}' \subseteq \mathcal{R}$. In this case, it follows that $\mathcal{X}' \subseteq \mathcal{X}$ and $\mathcal{C}' \subseteq \mathcal{C}$.
- b) A system (\mathcal{G}', K') , deterministic or stochastic, is a subsystem of a system (\mathcal{G}, K) if \mathcal{G}' is a subnetwork of \mathcal{G} and the rate functions agree on the reactions in \mathcal{R}' .
- c) The subnetwork \mathcal{G}^* given by the set of terminal reactions \mathcal{R}^* is the terminal network of \mathcal{G} . We denote $\mathcal{G}^* = (\mathcal{X}^*, \mathcal{C}^*, \mathcal{R}^*)$. Furthermore, the subsystem (\mathcal{G}^*, K^*) of (\mathcal{G}, K) is called the terminal system of (\mathcal{G}, K) .

Definition 2. The connected components of the reaction graph of the terminal network of \mathcal{G} are called terminal strongly connected component of \mathcal{G} . For any complex y in \mathcal{C}^* , we denote by (\mathcal{G}_y, K_y) the subsystem of \mathcal{G} whose reaction graph is the terminal strongly connected component containing y as node.

As an example, consider the mass-action system



Here, there are two terminal strongly connected components, which are $2A \rightleftharpoons 2B$ and $0 \rightleftharpoons C$. In particular, $(\mathcal{G}_{2A}, K_{2A})$ is equal to $(\mathcal{G}_{2B}, K_{2B})$ and is given by



Finally, if (\mathcal{G}, κ) is a mass-action system, any subsystems (\mathcal{G}', K') is a mass-action systems as well and can be denoted by (\mathcal{G}', κ') .

3 Deterministic reaction systems

In this section we will recapitulate the known characterisation of existence and uniqueness of positive equilibria in complex balanced systems and the connection between complex balanced systems and deficiency zero reaction networks. As we will show in the subsequent section, this characterisation can be fully translated into a similar characterisation for stochastic reaction networks.

3.1 Complex balanced systems

We start with a definition.

Definition 3. A deterministic reaction system (\mathcal{G}, K) is said to be complex balanced if there exists a positive complex balanced equilibrium, that is, a positive equilibrium point $c \in \mathbb{R}_+^n$ for the system (2.1), such that

$$\sum_{y' \in \mathcal{C}} \lambda_{y \rightarrow y'}(c) = \sum_{y' \in \mathcal{C}} \lambda_{y' \rightarrow y}(c) \quad \text{for all } y \in \mathcal{C}. \quad (3.1)$$

The name ‘complex balanced’ refers to the fact that the flow, at equilibrium, entering into the complex y equals the flow exiting from the complex. As an example, the mass-action system in (1.1) is complex balanced for any choice of (κ_1, κ_2) and $c = (\kappa_2, \kappa_1, \kappa_1)$ is a complex balanced equilibrium. The class of complex balanced systems is an extension of the class of detailed balanced mass-action systems [13, 10].

For mass-action systems, (3.1) becomes

$$\sum_{y' \in \mathcal{C}} \kappa_{y \rightarrow y'} c^y = \sum_{y' \in \mathcal{C}} \kappa_{y' \rightarrow y} c^{y'} \quad \text{for all } y \in \mathcal{C}, \quad (3.2)$$

with the convention that $\kappa_{y \rightarrow y'} = 0$ if $y \rightarrow y' \notin \mathcal{R}$.

In the case of mass-action kinetics, we extend Definition 3 to the stochastic case, by saying that a stochastic mass-action system (\mathcal{G}, κ) is complex balanced if the deterministic mass-action system (\mathcal{G}, κ) is

complex balanced. We might therefore refer to complex balanced mass-action systems without specifying whether they are stochastically or deterministically modelled.

The next theorem is a slight generalization of a classical result [13], which provides the backbone for the further characterisation. The generalization includes a property of non-negative equilibria

Theorem 3.1. *If a deterministic reaction system (\mathcal{G}, K) is complex balanced, then \mathcal{G} is weakly reversible. Moreover, if K is mass-action kinetics, then all equilibria are complex balanced, that is, they fulfil (3.2). Moreover, there exists exactly one positive equilibrium in each stoichiometric compatibility class, which is locally asymptotically stable.*

As we are not aware of a proof of this more general formulation, we provide one in Appendix B.

3.2 Deficiency zero statements

The *deficiency* plays an important role in the study of complex balanced systems. The deficiency of \mathcal{G} is defined as

$$\delta = m - \ell - s,$$

where m is the cardinality of \mathcal{C} , ℓ is the number of linkage classes of the reaction graph of \mathcal{G} and s is the dimension of the stoichiometric subspace S [13]. The definition hides the geometrical interpretation of the deficiency, which we now will explore.

Let $\{e_y\}_{y \in \mathcal{C}}$ be a basis of \mathbb{R}^m . Further, define

$$d_{y \rightarrow y'} = e_{y'} - e_y \quad \text{and} \quad \xi_{y \rightarrow y'} = y' - y$$

for $y \rightarrow y' \in \mathcal{R}$. Let $D = \text{span}(d_{y \rightarrow y'} | y \rightarrow y' \in \mathcal{R})$. Then $\dim D = m - \ell$ [13].

The space D is linearly isomorphic to the stoichiometric subspace S if and only if $\delta = 0$. Specifically, consider the homomorphism

$$\begin{aligned} \varphi: \quad \mathbb{R}^m &\rightarrow \mathbb{R}^n \\ e_y &\mapsto y. \end{aligned} \tag{3.3}$$

For $y \rightarrow y' \in \mathcal{R}$, we have $\varphi(d_{y \rightarrow y'}) = \xi_{y \rightarrow y'}$ and $\varphi|_D: D \rightarrow S$ is thus a surjective homomorphism. Therefore,

$$\dim \text{Ker } \varphi|_D = \dim D - s = m - \ell - s = \delta, \tag{3.4}$$

which implies that $\varphi|_D$ is an isomorphism if and only if $\delta = 0$. It further follows that the deficiency is a non-negative number.

We state here a useful Lemma on the deficiency of subnetworks.

Lemma 3.2. *Let \mathcal{G} be a reaction network with deficiency δ . Then, the deficiency of any subnetwork of \mathcal{G} is smaller than or equal to δ .*

Proof. Let $\mathcal{R}' \subseteq \mathcal{R}$ and let \mathcal{G}' be the corresponding subnetwork with deficiency δ' . Further, let D' and S' be the equivalent of D and S for \mathcal{G}' , respectively. By (3.4) and since D' is a subspace of D , we have $\delta' = \dim \text{Ker } \varphi|_{D'} \leq \dim \text{Ker } \varphi|_D = \delta$, which concludes the proof. \square

We next state two classical results which elucidate the connection between complex balanced systems and deficiency zero systems. A proof of the first and of the second result can be found in [13] and in [10], respectively. The results draw a connection between graphical and dynamical properties of a network. Theorem 3.4 is given here in a wider formulation than in [10] (see Appendix B for a proof).

Theorem 3.3. *The mass-action system (\mathcal{G}, κ) is complex balanced for any choice of κ if and only if \mathcal{G} is weakly reversible and its deficiency is zero.*

Theorem 3.4. *Consider a deterministic reaction system (\mathcal{G}, K) , and assume that the deficiency of \mathcal{G} is zero. If $x \in \mathbb{R}_0^n$ is an equilibrium point and $y \rightarrow y' \in \mathcal{R}$, then $\text{supp } y \subseteq \text{supp } x$ only if $y \rightarrow y'$ is terminal. Moreover, if K is mass-action kinetics with rate constants κ and $\text{supp } y \subseteq \text{supp } x$, then the projection of x onto the species space of \mathcal{G}_y is a complex balanced equilibrium of $(\mathcal{G}_y, \kappa_y)$.*

It follows from Theorem 3.4 that an equilibrium point satisfies (3.2) for the terminal system, though it is not necessarily a positive equilibrium of $(\mathcal{G}^*, \kappa^*)$. The deficiency zero theorem, in the following formulation, is a consequence of the three previous theorems:

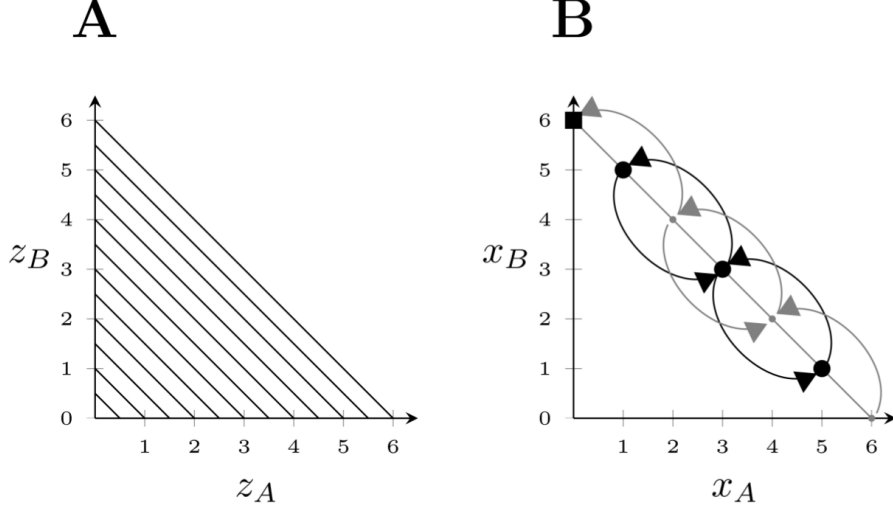


Figure 1: The figure shows some features of the reaction network $2A \rightarrow 2B$, and $A + 3B \rightarrow 3A + B$. (A) The stoichiometric compatibility classes are of the form $\{(z_A, z_B): z_A + z_B = \text{const.}\}$. (B) The two irreducible components on $\{(x_A, x_B): x_A + x_B = 6\}$ are shown (black circles and square), together with the possible transitions between the states. All states within a component are accessible from each other. The “square” component has no active reactions, both reactions are active on the “black circles” component. The grey states are transient states which are not in any irreducible component.

Theorem 3.5 (Deficiency zero theorem). *Consider a deterministic reaction system (\mathcal{G}, K) for which the deficiency is zero. Then the following statements hold:*

- i) *if \mathcal{G} is not weakly reversible, then there exists no positive equilibria;*
- ii) *if \mathcal{G} is weakly reversible and K is mass-action kinetics, then there exists within each stoichiometric compatibility class a unique positive equilibrium, which is asymptotically stable.*

The original formulation is richer than the one presented here [10].

4 Stochastic reaction systems

4.1 Classification of states and sets

To characterise the stochastic dynamics we introduce the following terminology.

Definition 4. *Let $\mathcal{G} = (\mathcal{X}, \mathcal{C}, \mathcal{R})$ be a reaction network.*

- a) *A reaction $y \rightarrow y' \in \mathcal{R}$ is active on $x \in \mathbb{N}^n$ if $x \geq y$.*
- b) *A state $u \in \mathbb{N}^n$ is accessible from a state $x \in \mathbb{N}^n$ if there is a sequence of $q \geq 0$ reactions $(y_j \rightarrow y'_j)_{j=1, \dots, q}$ such that*
 - (i) $u = x + \sum_{j=1}^q (y'_j - y_j)$,
 - (ii) $y_h \rightarrow y'_h$ is active on $x + \sum_{j=1}^{h-1} (y'_j - y_j)$ for all $1 < h \leq q$.

Definition 5. *Let \mathcal{G} be a reaction network. A non-empty set $\Gamma \subseteq \mathbb{N}^n$ is an irreducible component of \mathcal{G} if for all $x \in \Gamma$ and all $u \in \mathbb{N}^n$, u is accessible from x if and only if $u \in \Gamma$.*

Definition 6. *A reaction network \mathcal{G} is essential if the state space is a union of irreducible components. A reaction network \mathcal{G} is almost essential if the state space is a union of irreducible components except for a finite number of states.*

An essential network is also almost essential. A weakly reversible reaction network is essential [22]. Conditions for being essential can be found in [22, 11]. Any irreducible component is contained in some stoichiometric compatibility class, and a stoichiometric compatibility class may contain several irreducible components (Fig. 1B).

4.2 Stationary distribution

The stationary distribution π_Γ on an irreducible component Γ is unique, if it exists. It is characterised by the *master equation* [4]:

$$\sum_{y \rightarrow y' \in \mathcal{R}} \pi_\Gamma(x + y - y') \lambda_{y \rightarrow y'}(x + y - y') = \pi_\Gamma(x) \sum_{y \rightarrow y' \in \mathcal{R}} \lambda_{y \rightarrow y'}(x), \quad (4.1)$$

for all $x \in \Gamma$. Let $X(t)$ denote the stochastic process associated with the system. If $X(t_0)$ follows the law of π_Γ at time t_0 , then the distribution of $X(t)$ is π_Γ for all future times $t \geq t_0$. In this sense, the stationary distribution describes a state of equilibrium of the system. Moreover, if π_Γ exists, then

$$\lim_{t \rightarrow \infty} P(X(t) \in A) = \pi_\Gamma(A) \quad \text{for any } A \subseteq \Gamma, \quad (4.2)$$

provided that $X(0) \in \Gamma$ with probability one. As discussed in Section 1, a connection between mass-action complex balanced systems and their stationary distribution has been made in [2]:

Theorem 4.1. *Let (\mathcal{G}, κ) be a complex balanced mass-action system. Then, there exists a unique stationary distribution on every irreducible component Γ , and it is of the form*

$$\pi_\Gamma(x) = M_\Gamma^c \prod_{i=1}^n \frac{c_i^{x_i}}{x_i!} \quad \text{for } x \in \Gamma, \quad (4.3)$$

where c is a positive complex balanced equilibrium of (\mathcal{G}, κ) and M_Γ^c is a normalising constant.

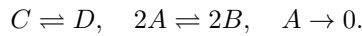
4.3 Parallel theorems for stochastic mass-action systems

In this section we derive stochastic statements corresponding to Theorem 3.1-3.5. Some of the proofs are deferred to Appendix B. We begin with a definition.

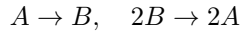
Definition 7. *For an irreducible component Γ , the set \mathcal{R}_Γ of active reactions on Γ consists of the reactions $y \rightarrow y' \in \mathcal{R}$ that are active on some $x \in \Gamma$. The subnetwork $\mathcal{G}_\Gamma = (\mathcal{X}_\Gamma, \mathcal{C}_\Gamma, \mathcal{R}_\Gamma)$ is called the Γ -network of \mathcal{G} and the subsystem $(\mathcal{G}_\Gamma, K_\Gamma)$ of (\mathcal{G}, K) is called the Γ -system of (\mathcal{G}, K) .*

The reactions that are active on Γ determine the dynamics of the stochastic system on Γ . To study the stationary distributions, it is therefore convenient to analyse the Γ -systems. Note that \mathcal{R}_Γ is empty if and only if Γ consists of a single state.

As an example, consider the deficiency zero network,



All molecules of A and B are irreversibly consumed through $A \rightarrow 0$ and $2B \rightarrow 2A$, thus the only active reactions on an irreducible component $\Gamma \neq \{0\}$ are $C \rightleftharpoons D$. The Γ -network is therefore $C \rightleftharpoons D$, which differs from the terminal system $C \rightleftharpoons D, 2A \rightleftharpoons 2B$. The next proposition states that for a deficiency zero reaction network $\mathcal{R}_\Gamma \subseteq \mathcal{R}^*$ for any irreducible component Γ . Note that Proposition 4.2 does not hold in general, for example,



has $\mathcal{R}_\Gamma = \mathcal{R}$ for any $\Gamma \neq \{0\}, \{(0, 1)\}$, while $\mathcal{R}^* = \emptyset$.

Proposition 4.2. *Let \mathcal{G} be a reaction network and Γ an irreducible component such that \mathcal{G}_Γ has deficiency zero. Then, \mathcal{G}_Γ is a subnetwork of \mathcal{G}^* . In particular, this is true if the deficiency of \mathcal{G} is zero.*

See Appendix B for a proof. Proposition 4.2 can be useful because \mathcal{R}_Γ might be difficult to find, especially if there are many complexes. On the other hand, terminal reactions are easily identified by means of the reaction graph. The next definitions are inspired by Definition 3.

Definition 8. Let (\mathcal{G}, K) be a stochastic reaction system. A stationary distribution π_Γ on an irreducible component Γ is said to be complex balanced if

$$\sum_{y \in \mathcal{C}_\Gamma} \pi_\Gamma(x - y' + y) \lambda_{y \rightarrow y'}(x - y' + y) = \sum_{y \in \mathcal{C}_\Gamma} \pi_\Gamma(x) \lambda_{y' \rightarrow y}(x) \quad \forall y' \in \mathcal{C}_\Gamma, x \in \Gamma. \quad (4.4)$$

For a mass-action system, (4.4) becomes

$$\sum_{y \in \mathcal{C}_\Gamma} \pi_\Gamma(x - y' + y) \kappa_{y \rightarrow y'} \frac{(x - y' + y)!}{(x - y')!} \mathbb{1}_{\{x \geq y'\}} = \sum_{y \in \mathcal{C}_\Gamma} \pi_\Gamma(x) \kappa_{y' \rightarrow y} \frac{x!}{(x - y')!} \mathbb{1}_{\{x \geq y'\}}$$

for any $y' \in \mathcal{C}_\Gamma$ and $x \in \Gamma$, with the convention that $k_{y \rightarrow y'} = 0$ if $y \rightarrow y' \notin \mathcal{R}_\Gamma$. In developing the theory for complex balanced equilibria in the deterministic setting, an important role is played by requiring positivity of the complex balanced equilibrium. Our aim is to introduce a similar concept for the stochastic systems. In the deterministic setting, if a state $z \in \mathbb{R}^n$ is positive then every rate function calculated on z is positive. We find inspiration from this to give the next definition:

Definition 9. An irreducible component Γ is positive if $\mathcal{G}_\Gamma = \mathcal{G}$.

Equivalently, an irreducible component Γ is *positive* if all reactions are active on Γ . The next definition follows naturally by analogy with the deterministic setting.

Definition 10. A stochastic reaction system (\mathcal{G}, K) is said to be stochastically complex balanced if there exists a complex balanced stationary distribution on a positive irreducible component.

If Γ is positive, then $\mathcal{C}_\Gamma = \mathcal{C}$ and a complex balanced stationary distribution on Γ satisfies (4.4) with \mathcal{C}_Γ replaced by \mathcal{C} . Note the similarity between Definition 10 and the definition of a complex balance equilibrium (Definition 3): the positivity of Γ plays the role of the positivity in Definition 3. Also note the close similarity between (3.1) and (4.4).

Theorem 4.3. Let (\mathcal{G}, K) be a stochastic reaction system, and let Γ be an irreducible component. If there exists a complex balanced stationary distribution π_Γ on Γ then \mathcal{G}_Γ is weakly reversible. Moreover, if K is mass-action kinetics with rate constants κ , there exists a complex balanced stationary distribution π_Γ on Γ if and only if the Γ -system of (\mathcal{G}, κ) is complex balanced. If this is the case, then π_Γ has the form

$$\pi_\Gamma(x) = M_\Gamma^c \prod_{i: S_i \in \mathcal{X}_\Gamma} \frac{c_i^{x_i}}{x_i!} \quad \text{for } x \in \Gamma, \quad (4.5)$$

where c is a positive complex balanced equilibrium of $(\mathcal{G}_\Gamma, \kappa_\Gamma)$ and M_Γ^c is a normalising constant.

The proof is in Appendix B. It is shown in [2] that the stationary distribution $\pi_\Gamma(x)$ is independent of the choice of complex balanced equilibrium c of the Γ -system, provided that it is positive. We are now ready to derive stochastic versions of Theorem 3.1-3.5. In addition, we will show that a stochastically complex balanced mass-action system is complex balanced and *vice versa*. Hence, we will show that the deterministic and stochastic systems are intimately connected. The next corollary is an analogue of Theorem 3.1.

Corollary 4.4. If a stochastic reaction system (\mathcal{G}, K) is stochastically complex balanced then \mathcal{G} is weakly reversible. Moreover, a mass-action system (\mathcal{G}, κ) is stochastically complex balanced if and only if it is complex balanced. If this is case, then on every irreducible component Γ there exists a unique stationary distribution π_Γ . Such π_Γ is a complex balanced stationary distribution and it has the form (4.3), where c is a positive complex balanced equilibrium of (\mathcal{G}, κ) .

Proof. If Γ is positive, then $(\mathcal{G}_\Gamma, K_\Gamma) = (\mathcal{G}, K)$. Therefore, by Theorem 4.3 if (\mathcal{G}, K) is stochastically complex balanced then \mathcal{G} is weakly reversible. Moreover, if K is mass-action kinetics with rate constants κ , it follows from Theorem 4.3 that there exists a complex balanced stationary distribution on Γ if and only if (\mathcal{G}, κ) is complex balanced. In this case, by Theorem 4.1, a stationary distribution exists on every irreducible component and it is of the form (4.3). By Theorem 4.3, it is a complex balanced stationary distribution. \square

Corollary 4.4 might be considered a stochastic version of Theorem 3.1, especially if (4.2) is taken to be equivalent to “asymptotic stability” for a deterministic equilibrium. Part of the corollary is known [2] (see also Theorem 4.1), and the whole corollary might therefore be considered as an extension of the result in [2] on mass-action systems. In this sense, Theorem 4.3 provides an even more general version, which deals with complex balanced subsystems of (\mathcal{G}, κ) .

We now state the parallel versions of Theorem 3.3-3.5 for the stochastic setting.

Corollary 4.5. *The mass-action system (\mathcal{G}, κ) is stochastically complex balanced for any choice of κ if and only if \mathcal{G} is weakly reversible and its deficiency is zero.*

Proof. The result is an immediate consequence of Corollary 4.4 and Theorem 3.3. \square

Theorem 4.6. *Consider a stochastic reaction system (\mathcal{G}, K) , and assume the deficiency of \mathcal{G} is zero. Let x be a state in an irreducible component Γ and let $y \rightarrow y'$ in \mathcal{R} . Then, $y \leq x$ only if $y \rightarrow y'$ is terminal. Moreover, if K is mass-action kinetics, then on Γ the stationary distribution has the form*

$$\pi_\Gamma(x) = M_\Gamma^c \prod_{i: S_i \in \mathcal{X}^*} \frac{c_i^{x_i}}{x_i!} \quad \text{for } x \in \Gamma, \quad (4.6)$$

where c is a positive complex balanced equilibrium for the terminal system, and M_Γ^c is a normalising constant.

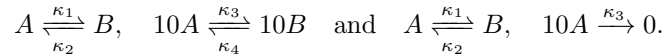
The proof is in Appendix B.

Theorem 4.7. *Consider a stochastic reaction system (\mathcal{G}, K) , and assume that the deficiency of \mathcal{G} is zero. Then the following statements hold:*

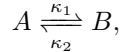
- i) *if \mathcal{G} is not weakly reversible, then there exist no positive irreducible components;*
- ii) *if \mathcal{G} is weakly reversible, then \mathcal{G} is essential, and if K is mass-action kinetics then there exists a unique stationary distribution on every irreducible component.*

The proof of the theorem is in Appendix B. In case (i), Theorem 4.6 provides the form of the stationary distribution. Hence we have characterised the stationary distribution for any deficiency zero reaction system, irrespectively whether it is complex balanced or not.

Example 1. Consider the two stochastic mass-action systems



The behaviours of the two corresponding deterministic systems differ substantially, while the behaviours of the stochastic systems are equivalent on the irreducible components $\Gamma_\theta = \{x \in \mathbb{N}^2: x_1 + x_2 = \theta\}$ with $0 \leq \theta < 10$ an integer. Indeed, in both cases the Γ_θ -system is



which is complex balanced (Theorem 3.3). It follows from Theorem 4.3 that the stationary distribution on Γ_θ is

$$\pi_\theta(x_1, x_2) = M_\theta \frac{\kappa_2^{x_1}}{x_1!} \frac{\kappa_1^{x_2}}{x_2!} \quad \text{for } (x_1, x_2) \in \Gamma_\theta,$$

for a suitable normalizing constant M_θ . The stationary distributions are complex balanced, but since Γ_θ is not positive in either of the two networks, we cannot conclude that the systems are stochastically complex balanced. Indeed, they are not for some choice of rate constants (Corollary 4.5).

Incidentally, note that the second network is not almost essential.

5 Product-form Poisson-like stationary distributions

The above results draw parallels between stochastic and deterministic reaction networks. If a mass-action system is (stochastically) complex balanced, then the stationary distribution on every irreducible component is a product-form Poisson-like distribution. Does the reverse statement hold true too? If the stationary distribution is a product-form Poisson-like distribution on some, or all irreducible components, does it follow that the system is complex balanced? In the spirit of the first part of the paper we would like to achieve a full characterisation of stochastic systems with product-form Poisson-like stationary distributions. However, even though the hypothesis of Theorem 5.1 below is rather general, a full characterisation seems hard to achieve.

Theorem 5.1. *Let \mathcal{G} be an almost essential reaction network, $\kappa \in \mathbb{R}_+^k$ a vector of rate constants and $c \in \mathbb{R}_+^n$ a vector with positive entries. The probability distribution $\pi_\Gamma: \Gamma \rightarrow (0, 1]$, defined by (4.3) is a stationary distribution for the stochastic mass-action system (\mathcal{G}, κ) for all irreducible components $\Gamma \subseteq \mathbb{N}^n$ of \mathcal{G} if and only if c is a complex balanced equilibrium for (\mathcal{G}, κ) .*

Proof. By Theorem 4.1, if $c > 0$ is a complex balanced equilibrium for (\mathcal{G}, κ) , then the stationary distribution on all irreducible components $\Gamma \subseteq \mathbb{N}^n$ is of the form (4.3).

Oppositely, assume that (4.3) is the stationary distribution on Γ for the stochastic mass-action system (\mathcal{G}, κ) , for all irreducible components Γ . Since \mathcal{G} is almost essential, there exists a constant K such that any states x with $\|x\| > K$ belongs to an irreducible component Γ . For any $x \in \mathbb{N}^n$, such that

$$\min_{S_i \in \mathcal{X}} x_i > \max_{y \rightarrow y' \in \mathcal{R}} (\|y\|_\infty + \|y'\|_\infty) + K, \quad (5.1)$$

we have that $x \geq y$ and $x - y' + y \geq y$ for all $y \rightarrow y' \in \mathcal{R}$. Then, since (4.3) is a stationary distribution and since x and $x + y - y'$ are in the same irreducible component for all $y \rightarrow y' \in \mathcal{R}$, we have from (4.1)

$$\sum_{y \rightarrow y' \in \mathcal{R}} \pi_\Gamma(x + y - y') \kappa_{y \rightarrow y'} \frac{(x + y - y')!}{(x - y')!} = \pi_\Gamma(x) \sum_{y \rightarrow y' \in \mathcal{R}} \kappa_{y \rightarrow y'} \frac{x!}{(x - y)!}, \quad (5.2)$$

for all $x \in \Gamma$ satisfying (5.1). Further, using (4.3), equation (5.2) becomes

$$\sum_{y \rightarrow y' \in \mathcal{R}} \frac{x!}{(x - y')!} \kappa_{y \rightarrow y'} c^{y - y'} = \sum_{y \rightarrow y' \in \mathcal{R}} \kappa_{y \rightarrow y'} \frac{x!}{(x - y)!},$$

which, by rearranging terms, leads to

$$\sum_{y' \in \mathcal{C}} \frac{x!}{(x - y')!} \sum_{y \rightarrow y' \in \mathcal{R}} \kappa_{y \rightarrow y'} c^{y - y'} = \sum_{y' \in \mathcal{C}} \frac{x!}{(x - y')!} \sum_{y' \rightarrow y \in \mathcal{R}} \kappa_{y' \rightarrow y}. \quad (5.3)$$

The equality holds for all $x \in \mathbb{N}^n$ satisfying (5.1), therefore the polynomials on the two sides of (5.3) are equal.

For any $y' \in \mathcal{C}$, let $p_{y'}(x)$ be the polynomial

$$p_{y'}(x) = \frac{x!}{(x - y')!}.$$

The monomial with maximal degree in $p_{y'}$ is $x^{y'}$, and these differ for all complexes $y' \in \mathcal{C}$. This implies that $p_{y'}$, $y' \in \mathcal{C}$, are linearly independent on \mathbb{R} , and thus, the polynomials on the two sides of (5.3) are equal if and only if

$$\sum_{y \in \mathcal{C}} \kappa_{y \rightarrow y'} c^{y - y'} = \sum_{y \in \mathcal{C}} \kappa_{y' \rightarrow y} \quad \text{for all } y' \in \mathcal{C}.$$

Hence, c is a complex balanced equilibrium for (\mathcal{G}, κ) and the proof is completed. \square

5.1 Relaxation of Assumptions in Theorem 5.1

To infer the existence of positive complex balanced equilibria in Theorem 5.1, the assumptions of the theorem could be weakened. Specifically, it is only required that (5.3) holds for a set of states whose geometry and cardinality allow us to conclude that the polynomials on the two sides of (5.3) are the same. For (5.3) to hold, we need x to be in a irreducible component and we require $x \geq y$ and $x - y' + y \geq y$ for all reactions $y \rightarrow y' \in \mathcal{R}$, as well as the stationary distribution evaluated in x and $x - y' + y$ to be of the form (4.3). If a state x satisfies this, we call it a *good state*.

A more general condition than being almost essential could be chosen case by case and depends on the monomials appearing in (5.3). For example, if the set of complexes coincides with the set of species, then the polynomials in (5.3) are linear and the existence of $n + 1$ *good states* in general position implies the existence of a positive complex balanced equilibrium. In general, let d be the total degree of the polynomials in (5.3). Then it is sufficient to have n lines in general position with more than $d + 1$ good states on each of them. Therefore, to conclude that a system is complex balanced it is sufficient to check the behaviour of a finite number of states, lying on a finite number of irreducible components. However, it follows from Examples 2 and 4 that the existence of arbitrarily many good states on a few irreducible components does not imply the existence of a positive complex balanced equilibrium in general. Finally, in order to postulate that the mass-action system is complex balanced, it is necessary that the vector c appearing in Theorem 5.1 is the same for every irreducible component, as shown in Example 5.

The following examples are also meant to give an idea of why it is hard to obtain a full characterization of stochastic mass-action systems with a product-form Poisson-like stationary distribution on some irreducible component.

Example 2. Let $\rho \in \mathbb{R}_+$ and let $\theta \geq 2$ be an integer. Consider the stochastic mass-action system

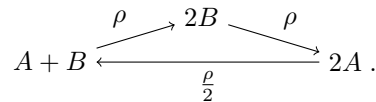


where $\kappa_1 = \rho(\theta - 1)$ and $\kappa_2 = \rho$ are the rate constants. The reaction network is almost essential. It is shown in Appendix C that the stationary distribution on the irreducible component $\Gamma_\theta = \{x \in \mathbb{N}^2 : x_1 + x_2 = \theta\}$ has the form (4.3) with $c = (1, 1)$, namely

$$\pi_\theta(x_1, x_2) = M_\theta \frac{1}{x_1! x_2!} \quad \text{for } (x_1, x_2) \in \Gamma_\theta, \quad (5.5)$$

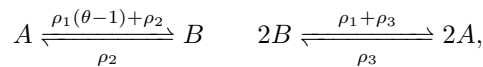
where M_θ is a normalising constant. However, the mass-action system is not complex balanced as the reaction network is not weakly reversible (Theorem 3.1). In particular, by Theorem 5.1, not all irreducible components can have a stationary distribution of the form (4.3) with $c = (1, 1)$. Trivially, the absorbing states $(0, 0)$ and $(0, 1)$ have it.

Additionally, we should point out that there is not an *equivalent* system on Γ (that is, a stochastic mass-action system with the same transition rate matrix on the states of Γ as (5.4)) which is complex balanced. Consider the case $\theta = 1$. Since the transition from $(0, 2)$ to $(2, 0)$ is possible according to (5.4), any equivalent mass-action system must contain the reaction $2B \rightarrow 2A$, with rate constant ρ . It can be further shown that any equivalent weakly reversible mass-action system must contain the connected component



This prevents the system from being complex balanced, since there is not a $c \in \mathcal{R}_+^2$ fulfilling (3.2) for the three complexes $2B$, $2A$ and $A + B$.

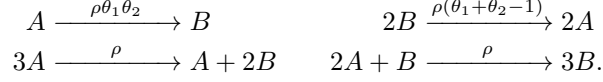
Example 3. Let $\rho_1, \rho_2, \rho_3 \in \mathbb{R}_+$ and let $\theta \geq 2$ be an integer. Consider the modification of Example 2 given by



which is weakly reversible. If we let $\rho_2 = 0$ and $\rho_3 = 0$, then the system reduces to that of Example 2 by removing the two reversible reactions. It can be shown that for any parameter choice, (5.5) is still

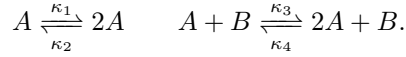
a stationary distribution on the irreducible component $\Gamma_\theta = \{x \in \mathbb{N}^2 : x_1 + x_2 = \theta\}$. However, for some choice of parameters the mass-action system is not complex balanced. This can be seen either by direct computation on the system of complex balance equations (3.2) or by noting that the deficiency of the network is 1, so there must be a choice of parameters which prevents positive complex balanced equilibria by Theorem 3.3. It can be further shown that irreducible components different from Γ do not possess a product-form Poisson-like stationary distribution.

Example 4. Consider the stochastic mass-action system with $\rho \in \mathbb{R}_+$ and θ_1, θ_2 two positive integers,

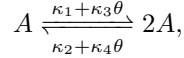


The reaction network is almost essential. For any $\theta \in \mathbb{N}$, consider the irreducible component $\Gamma_\theta = \{x \in \mathbb{N}^2 : x_1 + x_2 = \theta + 1\}$. Then π_{θ_1} and π_{θ_2} , defined as in (5.5), are the (unique) stationary distributions on the irreducible components Γ_{θ_1} and Γ_{θ_2} , respectively. For the relevant calculations see Appendix C. However, the mass-action system is not complex balanced, since the reaction network is not weakly reversible (Theorem 3.1).

Example 5. Theorem 5.1 can be also used to compute the stationary distribution of a stochastic mass-action system which behaves as a complex balanced system on the irreducible components. Consider the weakly reversible (and therefore essential) stochastic mass-action system



On every irreducible component $\Gamma_\theta = \{x \in \mathbb{N}^2 : x_2 = \theta\}$, $\theta \in \mathbb{N}$, the associated continuous time Markov chain, which describes the evolution of the counts of A , has the same distribution as the process associated with



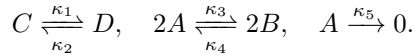
because the transition rates coincide. The latter system is complex balanced for any choice of rate constants. The stationary distribution has the form (Theorem 5.1)

$$\pi_\theta(x) = M_\theta \frac{1}{x!} \left(\frac{\kappa_2 + \kappa_4\theta}{\kappa_1 + \kappa_3\theta} \right)^x$$

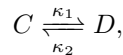
for some positive constant M_θ . The latter gives the stationary distribution of the original system as well. However, the rate of the Poisson distribution does depend on θ , in which case the original system cannot be complex balanced (Corollary 4.4). For the same reason the example does not contradict Theorem 5.1.

6 Applications

There are not many means to explicitly calculate the stationary distribution of a stochastic mass-action system. As an example, Theorem 4.3 can be used to determine the stationary distributions of mass-action systems like



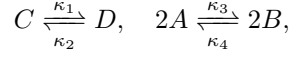
Indeed, for any irreducible component Γ different from $\{0\}$, the Γ -system is given by



which is weakly reversible and has deficiency zero, therefore it is complex balanced. Hence, the stationary distribution on Γ has the form

$$\pi_\Gamma(x) = M_\Gamma \frac{\kappa_2^{x_3} \kappa_1^{x_4}}{x_3! x_4!} \quad \text{for } x \in \Gamma,$$

where x_3 and x_4 denote the entries relative to C and D , respectively. Alternatively, since the terminal system is given by



Theorem 4.6 can be used to compute the stationary distribution. On every irreducible component Γ , it is given by

$$\pi_\Gamma(x) = \widetilde{M}_\Gamma \frac{(\sqrt{\kappa_4})^{x_1}}{x_1!} \frac{(\sqrt{\kappa_3})^{x_2}}{x_2!} \frac{\kappa_2^{x_3}}{x_3!} \frac{\kappa_1^{x_4}}{x_4!} \quad \text{for } x \in \Gamma,$$

which is equivalent to the previous formula since x_1 and x_2 are constantly 0 on all irreducible components.

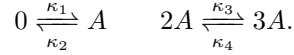
If the system does not fulfil the conditions of Theorem 4.3 and neither can be cast as a birth-death process, Theorem 5.1 might be useful. The following mass-action system is considered in [1]:



By Theorem 5.1, the stationary distribution cannot be Poisson. Indeed, it is given by the distribution of $Y = Y_1 + 2Y_2$, where Y_1 and Y_2 are two independent Poisson random variables with rates $\frac{\kappa_2}{\kappa_1}$ and $\frac{\kappa_2}{2\kappa_1}$, respectively. Hence,

$$\pi(x) = e^{-\frac{3\kappa_2}{2\kappa_1}} \sum_{\substack{i,j \in \mathbb{N} \\ x=i+2j}} \frac{1}{i!j!} \left(\frac{\kappa_2}{\kappa_1}\right)^i \left(\frac{\kappa_2}{2\kappa_1}\right)^j.$$

In [1], the following system is also considered:



It has the stationary distribution

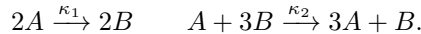
$$\pi(x) = M \prod_{i=1}^x \frac{\theta_1[(i-1)(i-2) + \theta_2]}{i(i-1)(i-2) + \theta_3 i} \quad \text{for } x \in \mathbb{N},$$

where $\theta_1 = \kappa_3/\kappa_4$, $\theta_2 = \kappa_1/\kappa_3$, $\theta_3 = \kappa_2/\kappa_4$ and $M = \pi(0)$ is a normalising constant. It is interesting that $\pi(x)$ is a Poisson distribution if and only if $\theta_2 = \theta_3$. In fact, and in accordance with our results, the mass-action system is complex balanced if and only if $\theta_2 = \theta_3$.

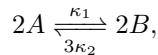
7 Discussion

Corollary 4.5 provides a characterisation of reaction networks that are stochastically complex balanced for any choice of rate constants. It is natural to wonder whether a stationary distribution of the form (4.3) on some irreducible component Γ for all choices of rate constants implies something specific about the Γ -system. If for specific form we intend deficiency zero and weakly reversible, this is not the case, as this is violated in Example 5. However, in Example 5 the system might be described *equivalently* by means of a weakly reversible deficiency zero system for any irreducible component. The question of whether this is always true remains open. We provide here two more examples.

Example 6. Consider the stochastic mass-action system



The underlying reaction network is considered in Figure 1. On the irreducible component $\Gamma = \{(1, 5), (3, 3), (5, 1)\}$, the Markov chain associated with the system has the same distribution as the Markov chain associated with

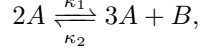


since the transition rates coincide. It is interesting to note that the dynamics of the two systems are different when they are deterministically modelled [8]. Due to Theorem 3.3, the latter system is complex balanced for any choice of rate constants. Therefore, by Theorem 5.1, the stationary distribution on Γ has the form (4.3) on both systems for any choice of rate constants. The same argument does not hold, in this case, for the other irreducible components.

Example 7. The same phenomenon as in Example 6 is observed in the stochastic mass-action system



On the irreducible component $\Gamma = \{(x_1, x_2) \in \mathbb{N}^2 : x_1 \geq 2, x_1 = x_2\}$, the Markov chain associated with the system has the same distribution as the Markov chain associated with



since the transition rates coincide, and the latter network is weakly reversible and has deficiency zero.

A Preliminary results

Here we state some preliminary results that will be needed in Appendix B.

Lemma A.1. *Let \mathcal{G} be a reaction network. If $y_1 \rightarrow y_2 \rightarrow \dots \rightarrow y_q$ is a directed path in the reaction graph of \mathcal{G} , and $x \geq y_1$, then $x + y_q - y_1$ is accessible from x .*

Proof. First, note that

$$x + \sum_{i=1}^{q-1} (y_{i+1} - y_i) = x + y_q - y_1.$$

It is sufficient to note that if $x \geq y_1$, then for any $1 \leq j \leq q-1$, we have

$$x + \sum_{i=1}^{j-1} (y_{i+1} - y_i) = x + y_j - y_1 \geq y_j.$$

This concludes the proof. \square

Lemma A.2. *Let Γ be an irreducible component such that \mathcal{G}_Γ has deficiency zero. Then, \mathcal{G}_Γ is weakly reversible. In particular, if \mathcal{G} has deficiency zero, \mathcal{G}_Γ has deficiency zero and is weakly reversible for every irreducible component Γ .*

Proof. If \mathcal{R}_Γ is empty then \mathcal{G}_Γ is weakly reversible and there is nothing to prove. Otherwise, if \mathcal{R}_Γ is non-empty, let $y_1 \rightarrow y'_1 \in \mathcal{R}_\Gamma$. By hypothesis, there exists a state x in Γ with $x \geq y_1$. This means that $x + \xi_{y_1 \rightarrow y'_1}$ is accessible from x . Moreover, since x belongs to an irreducible component Γ , we have that x is accessible from $x + \xi_{y_1 \rightarrow y'_1}$ as well, which implies that

$$x = x + \sum_{j=1}^q \xi_{y_j \rightarrow y'_j},$$

for a certain choice of $\xi_{y_j \rightarrow y'_j}$. In particular, $\sum_{j=1}^q \xi_{y_j \rightarrow y'_j} = 0$. By the hypothesis of deficiency zero, it follows that $\sum_{j=1}^q d_{y_j \rightarrow y'_j} = 0$, because φ , defined in (3.3), is an isomorphism between the spaces D and S associated with \mathcal{G}_Γ . Therefore,

$$\sum_{j=1}^q (e_{y'_j} - e_{y_j}) = \sum_{y \in \mathcal{C}_\Gamma} \alpha_y e_y = 0,$$

for some integers α_y . Since the vectors e_y are linearly independent, $\alpha_y = 0$ for all $y \in \mathcal{C}_\Gamma$. Hence, each e_y that appears in the sum, must appear at least twice, once with coefficient 1, once with -1 . Consequently, by iteratively reordering the terms $d_{y_j \rightarrow y'_j}$, the reactions $(y_j \rightarrow y'_j)_{j=1}^q$ form a union of directed closed paths in the reaction graph of \mathcal{G} . In particular, the reaction $y_1 \rightarrow y'_1$ is contained in a closed directed path of the reaction graph of \mathcal{G}_Γ , and since this is true for every reaction in \mathcal{R}_Γ , \mathcal{G}_Γ is weakly reversible. We conclude the proof by Lemma 3.2, since if \mathcal{G} has deficiency zero, so does every subnetwork of \mathcal{G} . \square

Lemma A.3. *Let \mathcal{G} be a weakly reversible reaction network, and let Γ be an irreducible component. Then, for any complex $y' \in \mathcal{C}_\Gamma$ we have*

$$\begin{aligned}\{y \in \mathcal{C} : y \rightarrow y' \in \mathcal{R}\} &= \{y \in \mathcal{C}_\Gamma : y \rightarrow y' \in \mathcal{R}_\Gamma\}, \\ \{y \in \mathcal{C} : y' \rightarrow y \in \mathcal{R}\} &= \{y \in \mathcal{C}_\Gamma : y' \rightarrow y \in \mathcal{R}_\Gamma\}.\end{aligned}$$

Proof. One inclusion is trivial, since $\mathcal{R}_\Gamma \subseteq \mathcal{R}$. For the other inclusion, fix $y' \in \mathcal{C}_\Gamma$. Suppose that there exists $x \in \Gamma$ with $x \geq y'$. It follows that any reaction $y' \rightarrow y \in \mathcal{R}$ is active on Γ , and therefore is contained in \mathcal{R}_Γ . Moreover, since \mathcal{G} is weakly reversible, for any reaction in \mathcal{R} of the form $y \rightarrow y'$, there exists a directed path in the reaction graph of \mathcal{G} from y' to y . Hence, by Lemma A.1, $x + y - y'$ is accessible from x , which implies that $x + y - y'$ is in Γ and that $y \rightarrow y'$ is in \mathcal{R}_Γ , since $x + y - y' \geq y$. Therefore, to conclude the proof it suffices to prove that there exists $x \in \Gamma$ with $x \geq y'$.

If it were no $x \in \Gamma$ with $x \geq y'$, then no reaction of the form $y' \rightarrow y$ would be in \mathcal{R}_Γ . Since $y' \in \mathcal{C}_\Gamma$, there exists a reaction of the form $y \rightarrow y'$. This means that there is $\tilde{x} \in \Gamma$, such that $\tilde{x} \geq y$. Hence, $\tilde{x} + y' - y$ is in Γ with $\tilde{x} + y' - y \geq y'$, which concludes the proof. \square

B Proofs

B.1 Proof of Theorem 3.1

It is proven in [13] that if a deterministic reaction system (\mathcal{G}, K) is complex balanced, then \mathcal{G} is weakly reversible. By [13], we also know that if K is mass-action kinetics, then all positive equilibria are complex balanced, and there exists exactly one positive equilibrium in each stoichiometric compatibility class, which is locally asymptotically stable. Therefore, to conclude the proof we only need to prove that in a complex balanced mass-action system (\mathcal{G}, κ) , the eventual equilibria on the boundary of \mathbb{R}^n are also complex balanced.

First of all note that any subsystem $(\mathcal{G}_L, \kappa_L)$ of (\mathcal{G}, κ) corresponding to a linkage classes L of \mathcal{G} is complex balanced. Indeed, the projection of a positive complex balanced equilibrium of (\mathcal{G}, κ) onto the space of the species of L satisfies (3.2) for any complex of \mathcal{G}_L , hence it is a positive complex balanced equilibrium of $(\mathcal{G}_L, \kappa_L)$.

Let c be an equilibrium point on the boundary. Consider a linkage class L of \mathcal{G} , and assume that $c_S > 0$ for any species S appearing in the linkage class. Then, the projection of c onto the species of L is a positive equilibrium of $(\mathcal{G}_L, \kappa_L)$, and therefore complex balanced. It follows that c satisfies (3.2) for any complex of L . Oppositely, assume that there exists a species appearing in the linkage class L , such that $c_S = 0$ (this can only happen on a boundary state). Remember that by mass-action kinetics, all the rates of reactions whose source complex contains S are zero. In particular, all the rates of reactions degrading S are zero. Consider a complex y in L that contains S . By weakly reversibility, there exists a reaction $y' \rightarrow y$ in L . If y' contains S , then $\lambda_{y' \rightarrow y}(c) = 0$. If y' does not contain S , then the reaction $y' \rightarrow y$ produces S . Since the rate of all reactions degrading S is zero at c and c is an equilibrium, then $\lambda_{y' \rightarrow y}(c)$ must be zero as well. By mass-action kinetics, this means that there exists a species $S' \neq S$ such that S' appears in y' and $c_{S'} = 0$. By iteratively applying the same argument with the new species S' and by weakly reversibility, we obtain that $\lambda_{y \rightarrow y'}(c) = 0$ for any reaction $y \rightarrow y'$ in L . It follows that c satisfies (3.2) for any complex in L , since the equation reduces to $0 = 0$. Equation (3.2) is therefore satisfied for any complex of \mathcal{G} and c is a complex balanced equilibrium. This concludes the proof. \square

B.2 Proof of Theorem 3.4

By [10, Theorem 6.1.2], if $x \in \mathbb{R}_0^n$ is an equilibrium point and $y \rightarrow y' \in \mathcal{R}$, then $\text{supp } y \subseteq \text{supp } x$ only if $y \rightarrow y'$ is terminal. Moreover, if $\text{supp } y \subseteq \text{supp } x$, then $\text{supp } \tilde{y} \subseteq \text{supp } x$ for every complex \tilde{y} of $\mathcal{G}_y = (\mathcal{X}_y, \mathcal{C}_y, \mathcal{R}_y)$.

Now, suppose that K is mass-action kinetics with rate constants κ , and that $\text{supp } y \subseteq \text{supp } x$ with $y \rightarrow y' \in \mathcal{R}$ (and therefore $y \rightarrow y' \in \mathcal{R}^*$). Consider

$$\tilde{\mathcal{R}} = \{\tilde{y} \rightarrow \tilde{y}' \in \mathcal{R} : \text{supp } \tilde{y} \subseteq \text{supp } x\}.$$

By the first part of the statement, the reaction graph of the subnetwork $\tilde{\mathcal{G}} = (\tilde{\mathcal{X}}, \tilde{\mathcal{C}}, \tilde{\mathcal{R}})$ is a union of terminal strongly connected components of \mathcal{G} , and therefore $\tilde{\mathcal{G}}$ is weakly reversible. Moreover, by Lemma

3.2, the deficiency of $\tilde{\mathcal{G}}$ is 0. It is not hard to see that the canonical projection of x onto the space of the species $\tilde{\mathcal{X}}$ is a positive equilibrium point of $(\tilde{\mathcal{G}}, \tilde{\kappa})$, and therefore complex balanced by Theorem 3.3. The proof is concluded by (3.2) and by noting that, for any complex $\tilde{y} \in \mathcal{C}_y$,

$$\begin{aligned}\{\tilde{y}' \in \tilde{\mathcal{C}}: \tilde{y} \rightarrow \tilde{y}' \in \tilde{\mathcal{R}}\} &= \{\tilde{y}' \in \mathcal{C}_y: \tilde{y} \rightarrow \tilde{y}' \in \mathcal{R}_y\}, \\ \{\tilde{y}' \in \tilde{\mathcal{C}}: \tilde{y}' \rightarrow \tilde{y} \in \tilde{\mathcal{R}}\} &= \{\tilde{y}' \in \mathcal{C}_y: \tilde{y}' \rightarrow \tilde{y} \in \mathcal{R}_y\}.\end{aligned}$$

□

B.3 Proof of Proposition 4.2

If \mathcal{R}_Γ is empty there is nothing to prove. Suppose that this is not the case. Since \mathcal{G}_Γ has deficiency zero, by Lemma A.2, it is weakly reversible. For any $y \rightarrow y' \in \mathcal{R}_\Gamma$, by definition there exists $x \in \Gamma$ such that $x \geq y$, which in turn implies $x + y' - y \geq y'$. Therefore, for any directed path in the reaction graph of \mathcal{G} that starts with $y \rightarrow y' \in \mathcal{R}_\Gamma$, all the reactions in the path belong to \mathcal{R}_Γ , by definition of \mathcal{R}_Γ . Since \mathcal{G}_Γ is weakly reversible, this can only happen if $\mathcal{R}_\Gamma \subseteq \mathcal{R}^*$, and this proves the first part of the statement. To conclude the proof, note that if the deficiency of \mathcal{G} is zero, then by Lemma 3.2 the deficiency of \mathcal{G}_Γ is zero as well. □

B.4 Proof of Theorem 4.3

For the first part of the statement, consider a continuous-time Markov chain $C_\Gamma(t)$ with state space $\Gamma \times \mathcal{C}$ and transition rate from (x, y) to $(x + y' - y, y')$ given by $\lambda_{y \rightarrow y'}(x)$ if $y \rightarrow y' \in \mathcal{R}_\Gamma$, and zero otherwise. The master equation for $C_\Gamma(t)$ is

$$\sum_{y \in \mathcal{C}_\Gamma} \tilde{\pi}(x - y' + y, y) \lambda_{y \rightarrow y'}(x - y' + y) = \sum_{y \in \mathcal{C}_\Gamma} \tilde{\pi}(x, y') \lambda_{y' \rightarrow y}(x) \quad \forall y' \in \mathcal{C}, x \in \Gamma,$$

with the convention that $\lambda_{y \rightarrow y'}(x) = 0$ if $y \rightarrow y' \notin \mathcal{R}_\Gamma$. By Definition 8, a stationary distribution for $C_\Gamma(t)$ exists and it is of the form $\tilde{\pi}(x, y) = M\pi(x)$, for a suitable normalising constant M . Since $\pi(x)$ is positive for any $x \in \Gamma$ (because it is a stationary distribution on an irreducible component), then by standard Markov chain theory, we have that for any two states $(x_1, y_1), (x_2, y_2) \in \Gamma \times \mathcal{C}$, if (x_2, y_2) is accessible from (x_1, y_1) , then (x_1, y_1) is accessible from (x_2, y_2) . Fix $y \rightarrow y' \in \mathcal{R}_\Gamma$ and $x \in \Gamma$ with $x \geq y$. Then, a directed path from $(x + y' - y, y')$ to (x, y) exists in the graph associated with $C_\Gamma(t)$. The second components of the form y of the states in the path, by construction, determine a directed path in the reaction graph of \mathcal{G}_Γ from y' to y . Hence, any reaction $y \rightarrow y' \in \mathcal{R}_\Gamma$ is contained in a closed directed path, which means that \mathcal{G}_Γ is weakly reversible.

Assume now that K is mass-action kinetics with rate constants κ and that c is a positive complex balanced equilibrium of (\mathcal{G}, κ) . Then, by Theorem 4.1, there exists a (unique) stationary distribution on Γ of the form (4.3). If a species S_j is not in \mathcal{X}_Γ , then the value of x_j is constant for any $x \in \Gamma$, and (4.5) can be obtained from (4.3) by modifying the normalising constant.

By Theorem 3.1 and Lemma A.3, we have that

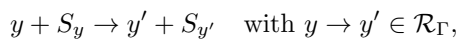
$$\sum_{y \in \mathcal{C}_\Gamma} c^{y-y'} \kappa_{y \rightarrow y'} = \sum_{y \in \mathcal{C}_\Gamma} \kappa_{y' \rightarrow y} \quad \forall y' \in \mathcal{C}_\Gamma,$$

with $\kappa_{y \rightarrow y'} = 0$ if $y \rightarrow y' \notin \mathcal{R}_\Gamma$. Therefore, for any $y' \in \mathcal{C}_\Gamma$ and $x \in \Gamma$,

$$\frac{1}{(x - y')!} \sum_{y \in \mathcal{C}_\Gamma} c^{x+y-y'} \kappa_{y \rightarrow y'} \mathbb{1}_{\{x \geq y'\}} = \frac{1}{(x - y')!} \sum_{y \in \mathcal{C}_\Gamma} c^x \kappa_{y' \rightarrow y} \mathbb{1}_{\{x \geq y'\}},$$

which leads to (4.4), since π is of the form (4.3).

To prove the converse we first introduce a new stochastic mass-action system $(\hat{\mathcal{G}}_\Gamma, \hat{\kappa}_\Gamma)$, which is given by the reactions of the form



where S_y are fictitious species in one to one correspondence with the complexes \mathcal{C}_Γ . The rate constant of the reaction $y + S_y \rightarrow y' + S_{y'}$ is given by $\kappa_{y \rightarrow y'}$. It is not difficult to see that the sum of the fictitious species is conserved for any possible trajectory. Moreover, since any directed path $y_1 \rightarrow y_2 \rightarrow \dots y_q$ in the reaction graph of \mathcal{G} corresponds to a directed path $y_1 + S_{y_1} \rightarrow y_2 + S_{y_2} \rightarrow \dots y_q + S_{y_q}$ in the reaction graph of $\hat{\mathcal{G}}_\Gamma$, we have that $\hat{\mathcal{G}}_\Gamma$ is weakly reversible by the first part of the proof.

Consider the set

$$\Upsilon = \{(x, \hat{x}) \in \mathbb{N}^n \times \mathbb{N}^m : x \in \Gamma, \|\hat{x}\|_1 = 1\}.$$

Every state in Υ is of the form $(x, S_y) \in \mathbb{N}^{n+m}$, where $x \in \Gamma$ and S_y is considered as the vector in \mathbb{N}^m with entry 1 in the position corresponding to the species S_y and 0 otherwise. Since Γ is an irreducible component of \mathcal{G} and the sum of the fictitious species is conserved, no state outside Υ is accessible from any state in Υ , according to $\hat{\mathcal{G}}_\Gamma$. Moreover, the master equation on Υ can be written as

$$\begin{aligned} \sum_{y \in \mathcal{C}_\Gamma} \hat{\pi}(x - y' + y, S_y) \kappa_{y \rightarrow y'} \frac{(x - y' + y)!}{(x - y')!} \mathbb{1}_{\{x \geq y'\}} \\ = \sum_{y' \in \mathcal{C}_\Gamma} \hat{\pi}(x, S_{y'}) \kappa_{y' \rightarrow y} \frac{x!}{(x - y')!} \mathbb{1}_{\{x \geq y'\}} \quad \forall y' \in \mathcal{C}, x \in \Gamma. \end{aligned} \quad (\text{B.1})$$

If we choose $\hat{\pi}(x, \hat{x}) = M\pi(x)$ for some positive constant M , then the master equation (B.1) is satisfied due to Definition 8. Therefore, if M is chosen as a suitable normalising constant, $\hat{\pi}(x, z) = M\pi(x)$ is a stationary distribution on Υ .

Consider the linear homomorphism φ as defined in (3.3), for the reaction network $\hat{\mathcal{G}}_\Gamma$. Let $|\cdot|$ denote the cardinality of a set, and note that $|\hat{\mathcal{C}}_\Gamma| = |\mathcal{C}_\Gamma| = m_\Gamma$. For any vector e_y of the basis of \mathbb{R}^{m_Γ} , we have $\varphi(e_y) = (y, S_y)$. Since the vectors (y, S_y) with $y \in \mathcal{C}_\Gamma$ are linear independent, φ is an isomorphism and the deficiency of $\hat{\mathcal{G}}_\Gamma$ is 0.

Since $\hat{\mathcal{G}}_\Gamma$ is a deficiency zero weakly reversible reaction network, it follows from Theorem 3.3 that the mass-action system $(\hat{\mathcal{G}}_\Gamma, \kappa)$ is complex balanced. Therefore, by Theorem 4.1, we have that $\hat{\pi}$ has the form

$$\hat{\pi}(x, \hat{x}) = M_{\hat{\Gamma}}^{(c, \hat{c})} \frac{c^x \hat{c}^{\hat{x}}}{x! \hat{x}!},$$

for a positive complex balanced equilibrium (c, \hat{c}) , on any irreducible component $\hat{\Gamma}$ contained in Υ . Since $\hat{\pi}(x, \hat{x}) = M\pi(x)$ does not depend on \hat{x} , we have

$$\hat{\pi}(x, \hat{x}) = M_\Gamma^c \frac{c^x}{x!},$$

for any $(x, \hat{x}) \in \Upsilon$.

Fix a complex $y' \in \mathcal{C}_\Gamma$. Since \mathcal{G}_Γ is weakly reversible, there exists a reaction $y' \rightarrow y$ that is active on Γ . Fix $x \in \Gamma$ such that $x \geq y'$. Then for any $y \rightarrow y' \in \mathcal{R}_\Gamma$ we have $x - y' + y \geq y$. If we plug the formula for $\hat{\pi}(x, \hat{x})$ in (B.1) for our choice of x and y' , we obtain

$$\sum_{y \in \mathcal{C}_\Gamma} M_\Gamma^c \frac{c^{x-y'+y}}{(x - y' + y)!} \kappa_{y \rightarrow y'} \frac{(x - y' + y)!}{(x - y')!} = \sum_{y \in \mathcal{C}_\Gamma} M_\Gamma^c \frac{c^x}{x!} \kappa_{y' \rightarrow y} \frac{x!}{(x - y')!},$$

which leads to

$$\sum_{y \in \mathcal{C}_\Gamma} c^{y-y'} \kappa_{y \rightarrow y'} = \sum_{y \in \mathcal{C}_\Gamma} \kappa_{y' \rightarrow y}.$$

The proof is concluded by the fact that the above holds for any fixed $y' \in \mathcal{C}_\Gamma$, which means that c is a positive complex balanced equilibrium of $(\mathcal{G}_\Gamma, \kappa_\Gamma)$. \square

B.5 Proof of Theorem 4.6

By Lemma A.2, \mathcal{G}_Γ is weakly reversible. Moreover, for $y \rightarrow y' \in \mathcal{R}_\Gamma$, if $x \geq y$ then $x + y' - y \geq y'$. This implies that for any directed path in the reaction graph of \mathcal{G} that starts with $y \rightarrow y' \in \mathcal{R}_\Gamma$, all the reactions in the path belong to \mathcal{R}_Γ , by definition of \mathcal{R}_Γ . Since \mathcal{G}_Γ is weakly reversible, every directed

path in the reaction graph of \mathcal{G} that starts with $y \rightarrow y' \in \mathcal{R}_\Gamma$ is contained in a closed directed path. This implies that $\mathcal{R}_\Gamma \subseteq \mathcal{R}^*$, and proves the first part of the statement.

Now assume that K is mass-action kinetics with rate constants κ . If the deficiency of \mathcal{G} is zero, then by Lemma 3.2 the deficiency of the terminal network is zero as well. Moreover, \mathcal{G}^* is weakly reversible by definition, thus by Theorem 3.3 $(\mathcal{G}^*, \kappa^*)$ is complex balanced for any choice of rate constants κ^* .

Let $X(t)$ be the stochastic process associated with (\mathcal{G}, κ) . By the first part of the statement, on Γ only terminal reactions take place and these involve a subset of the species only. Without loss of generality, we can assume that \mathcal{X}^* is constituted by the first n^* species of \mathcal{X} . Therefore, Γ is of the form $\Gamma^* \times \{v\}$, with $\Gamma^* \subseteq \mathcal{R}^{n^*}$ and $v \in \mathbb{R}^{n-n^*}$. Moreover, we have that on Γ^* , the projection $X^*(t) = (X_1(t), \dots, X_{n^*}(t))$ is distributed as the process associated with $(\mathcal{G}^*, \kappa^*)$, for which Γ^* is an irreducible component. Let c be a positive complex balanced equilibrium for $(\mathcal{G}^*, \kappa^*)$. Hence, by Theorem 4.1 or Corollary 4.4, the stationary distribution of the process $X(t) = (X^*(t), v)$ on Γ is of the form (4.6). \square

B.6 Proof of Theorem 4.7

For the first part, we prove that if an irreducible component Γ is positive, then \mathcal{G} is weakly reversible. This simply follows from Lemma A.2: indeed, by the lemma, \mathcal{G}_Γ is weakly reversible and since Γ is positive, $\mathcal{G}_\Gamma = \mathcal{G}$.

To prove the second part, we have to show that a weakly reversible reaction network is essential, and this is done in [22]. Moreover, a deficiency zero weakly reversible mass-action system is complex balanced, and the proof is concluded by Theorem 4.1 or Corollary 4.4. \square

C Calculations for Examples 2 and 4

In Example 2, we claim that the stationary distribution on the irreducible component $\Gamma_\theta = \{x \in \mathbb{N}^2 : x_1 + x_2 = \theta\}$ has the form

$$\pi_\theta(x_1, x_2) = M_\theta \frac{1}{x_1!x_2!} \quad \text{for } (x_1, x_2) \in \Gamma_\theta.$$

To prove this, it is sufficient to show that π_θ satisfies the master equation for every point (x_1, x_2) of Γ_θ . The master equation on (x_1, x_2) is given by

$$\begin{aligned} \rho \pi_\theta(x_1 + 1, x_2 - 1)(\theta - 1)(x_1 + 1) \mathbb{1}_{\{x_2 \geq 1\}} + \rho \pi_\theta(x_1 - 2, x_2 + 2) \frac{(x_2 + 2)!}{x_2!} \mathbb{1}_{\{x_1 \geq 2\}} \\ = \rho \pi_\theta(x_1, x_2) \left((\theta - 1)x_1 \mathbb{1}_{\{x_1 \geq 1\}} + \frac{(x_2)!}{(x_2 - 2)!} \mathbb{1}_{\{x_2 \geq 2\}} \right). \end{aligned}$$

By plugging in the formula for π_θ and after dividing by ρ and M_θ we obtain

$$\frac{1}{x_1!x_2!} [x_2(\theta - 1) + x_1(x_1 - 1)] = \frac{1}{x_1!x_2!} [x_1(\theta - 1) + x_2(x_2 - 1)].$$

If we multiply by $x_1!x_2!$ and substitute $\theta = x_1 + x_2$, it follows that

$$x_2(x_1 + x_2 - 1) + x_1(x_1 - 1) = x_1(x_1 + x_2 - 1) + x_2(x_2 - 1),$$

that is

$$x_1x_2 + x_2^2 - x_2 + x_1^2 - x_1 = x_1^2 + x_1x_2 - x_1 + x_2^2 - x_2,$$

which always holds true because the terms cancel each other.

In Example 4, we change the notation to $\Gamma_\theta = \{x \in \mathbb{N}^2 : x_1 + x_2 = \theta + 1\}$. Then we claim that the stationary distributions on the irreducible components Γ_{θ_1} and Γ_{θ_2} are π_{θ_1} and π_{θ_2} , respectively, where as before

$$\pi_\theta(x_1, x_2) = M_\theta \frac{1}{x_1!x_2!} \quad \text{for } (x_1, x_2) \in \Gamma_\theta.$$

We prove that π_{θ_1} is the stationary distribution on Γ_{θ_1} . The case with θ_2 is analogue. We prove the result by consider the master equation for π_{θ_1} on a point $(x_1, x_2) \in \Gamma_{\theta_1}$, which is as following:

$$\begin{aligned}
& \rho\pi_{\theta_1}(x_1+1, x_2-1)\theta_1\theta_2(x_1+1)\mathbb{1}_{\{x_2 \geq 1\}} \\
& + \rho\pi_{\theta_1}(x_1-2, x_2+2)(\theta_1+\theta_2-1)\frac{(x_2+2)!}{x_2!}\mathbb{1}_{\{x_1 \geq 2\}} \\
& + \rho\pi_{\theta_1}(x_1+2, x_2-2)\frac{(x_1+2)!}{(x_1-1)!}\mathbb{1}_{\{x_1 \geq 1, x_2 \geq 2\}} \\
& + \rho\pi_{\theta_1}(x_1+2, x_2-2)\frac{(x_1+2)!(x_2-2)!}{x_1!(x_2-3)!}\mathbb{1}_{\{x_1 \geq 0, x_2 \geq 3\}} \\
& = \rho\pi_{\theta_1}(x_1, x_2)\theta_1\theta_2x_1\mathbb{1}_{\{x_1 \geq 1\}} + \rho\pi_{\theta_1}(x_1, x_2)(\theta_1+\theta_2-1)\frac{x_2!}{(x_2-2)!}\mathbb{1}_{\{x_2 \geq 2\}} \\
& + \rho\pi_{\theta_1}(x_1, x_2)\frac{x_1!}{(x_1-3)!}\mathbb{1}_{\{x_1 \geq 3\}} + \rho\pi_{\theta_1}(x_1, x_2)\frac{x_1!x_2!}{(x_1-2)!(x_2-1)!}\mathbb{1}_{\{x_1 \geq 2, x_2 \geq 1\}}.
\end{aligned}$$

As we did for the previous calculations, we plug in the expression for π_{θ_1} , then divide by M_{θ_1} , ρ and multiply by $x_1!x_2!$. We obtain

$$\begin{aligned}
& \theta_1\theta_2x_2 + (\theta_1+\theta_2-1)x_1(x_1-1) + x_1x_2(x_2-1) + x_2(x_2-1)(x_2-2) \\
& = \theta_1\theta_2x_1 + (\theta_1+\theta_2-1)x_2(x_2-1) + x_1(x_1-1)(x_1-2) + x_1(x_1-1)x_2.
\end{aligned}$$

Finally, by substituting θ_1 with x_1+x_2-1 and by performing the calculations, we obtain $0=0$, which means that the above equation is satisfied.

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